1135-65-1813 **Lin Lin*** (linlin@berkeley.edu), **Wei Hu** and **Chao Yang**. *Projected Commutator DIIS method for linear and nonlinear eigenvalue problems.*

The commutator direct inversion of the iterative subspace (commutator DIIS or C-DIIS) method developed by Pulay in the 1980s is an efficient and the most widely used scheme for solving nonlinear eigenvalue problems in quantum chemistry. However, for large matrices this method is not practical due to the need of explicit construction of the projector and the commutator. I will discuss a newly developed Projected Commutator DIIS method (PC-DIIS) method to accelerate nonlinear eigenvalue problems and even certain linear eigenvalue problems with much reduced cost. The PC-DIIS method has been successfully applied to accelerate hybrid functional density functional theory calculations in quantum chemistry. (Joint work with Wei Hu and Chao Yang) (Received September 25, 2017)